# A Phase-Fitted Runge-Kutta-Nyström method for the Numerical Solution of Initial Value Problems with Oscillating Solutions

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**Abstract**

A new Runge-Kutta-Nyström method, with phase-lag of order infinity, for the integration of second-order periodic initial-value problems is developed in this paper. The new method is based on the Dormand and Prince Runge-Kutta-Nyström method of algebraic order four[1]. Numerical illustrations indicate that the new method is much more efficient than the classical one.

*Key words:* Runge-Kutta-Nyström methods; Phase-fitted; Initial-value problems; Phase-lag infinity
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## 1. Introduction

In this paper we study a special Runge-Kutta-Nyström method of Dormand *et al.*[1] for integrating systems of ODEs of the form

$$\frac{d^2u(t)}{dt^2} = f(t, u(t)) \tag{1}$$

for which it is known in advantage that their solution is periodic or oscillating.

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Several authors in their papers (*for example see* [3,7-10]) have developed Runge-Kutta-Nyström methods with the purpose of making the phase-lag of the method smaller.

The *phase-lag* of a method, first defined by Brusa and Nigro [2] at 1980. Van der Houwen and Sommeijer [3] proposed second-order $m$-stage methods (with $m = 4, 5, 6$) and phase-lag order $q = 6, 8, 10$ respectively. They also derived some third-order methods with phase-lag order $6, 8, 10$. In [3, 5] Chawla and Rao have constructed Numerov-type methods with minimal phase-lag for the numerical integration of second-order initial-value problems. Simos *et al*. [8] obtain fourth-order Runge-Kutta-Nyström with minimal phase-lag of order eigth. He also derived in [9] a Runge-Kutta-Fehlberg method of order infinity.

In the present paper and based on the requirements of infinite order of phase-lag, we will construct a phase-fitted four-stage Runge-Kutta-Nyström which is based on the coefficients of the well-known Runge-Kutta-Nyström Dormand *et al*. [1] method of algebraic order 4.

## 2. Phase lag analysis for Runge-Kutta-Nyström methods

The general m-stage method for the equation

$$\frac{d^2u(t)}{dt^2} = f(t, u(t)) \tag{2}$$

is of the form

$$\begin{aligned} u_n{}^{(0)} &= u_{n-1}, & u_n^{(i)} &= u_{n-1} + h\hat{u}_{n-1} + h^2 \sum_{j=1}^{i} b_j f_j, \\ u_n &= u_n^{(m)}, & \hat{u}_n &= \hat{u}_{n-1} + h \sum_{j=1}^{i} \hat{b}_j f_j, \end{aligned} \tag{3}$$

where

$$f_i = f(t_{n-1} + c_i h, u_{n-1} + hc_i\hat{u}_{n-1} + h^2 \sum_{j=1}^{i-1} \alpha_{i,j} u_n^{(j)}) \tag{4}$$

and $c_1 = 0$ and $c_m = 1$

The above expressions are presented using the well-known Butcher table, given below:

| | | | | | |
|---|---|---|---|---|---|
| $0$ | | | | | |
| $c_2$ | $\alpha_{21}$ | | | | |
| $c_3$ | $\alpha_{31}$ | $\alpha_{32}$ | | | |
| $\vdots$ | $\vdots$ | $\vdots$ | | | |
| $c_m$ | $\alpha_{m,1}$ | $\alpha_{m,2}$ | $\ldots$ | $\alpha_{m,m-1}$ | |
| | $b_1$ | $b_2$ | $\ldots$ | $b_{m-1}$ | $b_m$ |
| | $\hat{b}_1$ | $\hat{b}_2$ | $\ldots$ | $\hat{b}_{m-1}$ | $\hat{b}_m$ |

Table 1: m-stage Runge-Kutta-Nystöm method

In order to develop the new method, we use the test equation,

$$\frac{d^2u(t)}{dt^2} = (iv)^2u(t) \Longrightarrow u''(t) = -v^2u(t), \qquad v \in R \tag{5}$$

By applying the general method (3) to the test equation (5) we obtain the numerical solution

$$\left[\begin{array}{c} u_n \\ h\hat{u}_n \end{array}\right] = D^n \left[\begin{array}{c} u_0 \\ h\hat{u}_0 \end{array}\right], \quad D = \left[\begin{array}{cc} A(z^2) & B(z^2) \\ A'(z^2) & B'(z^2) \end{array}\right], \quad z = vh, \tag{6}$$

where $A, B, A', B'$ are polynomials in $z^2$, completely determined by the parameters of method (3)

The exact solution of (5) is given by

$$u(t_n) = \sigma_1[exp(iv)]^n + \sigma_2[exp(-iv)]^n, \tag{7}$$

where

$$\sigma_{1,2} = \frac{1}{2}[u_0 \pm \frac{(i\hat{u}_0)}{v}] \quad or \quad \sigma_{1,2} = |\sigma|exp(\pm i\chi).$$

Substituting in (7), we have

$$u(t_n) = 2|\sigma|cos(\chi + nz). \tag{8}$$

Furthermore we assume that the eigenvalues of $D$ are $\varrho_1, \varrho_2$, and the consequent eigenvectors are $[1, v_1]^T, [1, v_2]^T$,
where $v_i = A'/(\rho_i - B'), i = 1, 2$. The numerical solution of (5) is

$$u_n = c_1\rho_1^n + c_2\rho_2^n, \tag{9}$$

where

$$c_1 = -\frac{v_2 u_0 - h\hat{u}_0}{v_1 - v_2}, \quad c_2 = -\frac{v_1 u_0 - h\hat{u}_0}{v_1 - v_2}.$$

If $\rho_1, \rho_2$ are complex conjugate, then $c_{1,2} = |c|exp(\pm iw)$ *and* $\rho_{1,2} = |\rho|exp(\pm ip)$. By substituting in (9), we have

$$u_n = 2|c||\rho|^n cos(w + np). \tag{10}$$

From equations (8) and (10) we take the following definition.

***Definition* 1.** *(Phase-lag). Apply the RKN method (3) to the general method (5). Then we define the phase-lag $\Phi(z) = z - p$. If $\Phi(z) = O(z^{q+1})$, then the RKN method is said to have phase-lag order $q$.*

In addition, the quantity $a(z) = 1 - |\rho|$ is called *amplification error.*

Let us denote

$$\begin{aligned} R(z^2) &= tr(D) = A(z^2) + B'(z^2) \\ Q(z^2) &= det(D) = A(z^2)B'(z^2) - A'(z^2)B(z^2) \end{aligned} \tag{11}$$

where $z = vh$. From Definition 1 it follows that

$$\Phi(z) = z - arcoss\Big(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\Big), \qquad |\rho| = \sqrt{Q(z^2)}. \tag{12}$$

We can also put forward an alternative definition for the case of infinite order of phase lag.

***Definition* 2.** *(Phase-lag of order infinity). To obtain phase-lag of order infinity the relation $\Phi(z) = z - arccos\Big(\frac{R(z^2)}{2\sqrt{Q(z^2)}}\Big) = 0$ must hold.*

## 3. Derivation of the new Runge-Kutta-Nyström method

In this section we construct a 4-stage explicit Runge-Kutta-Nyström method (presented in Table 1), based on $R(z^2)$ and $Q(z^2)$. Now let us rewrite R and Q in the following form

$$\begin{aligned} R(z^2) &= 2 - r_1 z^2 + r_2 z^4 - r_3 z^6 + \ldots + r_i z^{2i} = 0 \\ Q(z^2) &= 1 - q_1 z^2 + q_2 z^4 - q_3 z^6 + \ldots + q_i z^{2i} = 0 \end{aligned} \tag{13}$$

By computing the polynomials $A, B, A', B'$ and therefore $R$ and $Q$ in terms of RKN parameters we obtain the following expressions

$$A(z^2) = 1 + b_4 a_{4,3} a_{3,2} a_{2,1} z^8 + (-b_4 a_{4,2} a_{2,1} - b_3 a_{3,2} a_{2,1} - b_4 a_{4,3} a_{3,1} - b_4 a_{4,3} a_{3,2}) z^6 + (b_2 a_{2,1} + b_4 a_{4,1} + b_4 a_{4,2} + b_3 a_{3,1} + b_4 a_{4,3} + b_3 a_{3,2}) z^4 + (-b_4 - b_1 - b_3 - b_2) z^2$$

$$B(z^2) = 1 - b_4 a_{4,3} a_{3,2} c_2 z^6 + (b_4 a_{4,3} c_3 + b_4 a_{4,2} c_2 + b_3 a_{3,2} c_2) z^4 + (-b_3 c_3 - b_4 c_4 - b_2 c_2) z^2$$

$$A'(z^2) = \hat{b}_4 a_{4,3} a_{3,2} a_{2,1} z^8 + (-\hat{b}_3 a_{3,2} a_{2,1} - \hat{b}_4 a_{4,3} a_{3,1} - \hat{b}_4 a_{4,3} a_{3,2} - \hat{b}_4 a_{4,2} a_{2,1}) z^6 + (\hat{b}_2 a_{2,1} + \hat{b}_3 a_{3,1} + \hat{b}_3 a_{3,2} + \hat{b}_4 a_{4,1} + \hat{b}_4 a_{4,2} + \hat{b}_4 a_{4,3}) z^4 + (-\hat{b}_4 - \hat{b}_2 - \hat{b}_1 - \hat{b}_3) z^2$$

$$B'(z^2) = 1 - \hat{b}_4 a_{4,3} a_{3,2} c_2 z^6 + (\hat{b}_4 a_{4,3} c_3 + \hat{b}_4 a_{4,2} c_2 + \hat{b}_3 a_{3,2} c_2) z^4 + (-\hat{b}_3 c_3 - \hat{b}_4 c_4 - \hat{b}_2 c_2) z^2$$

$$R(z^2) = 2 + b_4 a_{4,3} a_{3,2} a_{2,1} z^8 + (-b_3 a_{3,2} a_{2,1} - b_4 a_{4,3} a_{3,2} - b_4 a_{4,2} a_{2,1} - \hat{b}_4 a_{4,3} a_{3,2} c_2 - b_4 a_{4,3} a_{3,1}) z^6 + (b_2 a_{2,1} + b_3 a_{3,2} + b_4 a_{4,3} + \hat{b}_3 a_{3,2} c_2 + \hat{b}_4 a_{4,3} c_3 + \hat{b}_4 a_{4,2} c_2 + b_3 a_{3,1} + b_4 a_{4,1} + b_4 a_{4,2}) z^4 + (-b_3 - b_2 - \hat{b}_3 c_3 - \hat{b}_4 c_4 - \hat{b}_2 c_2 - b_4 - b_1) z^2$$

$$\begin{aligned} Q(z^2) = 1 &+ (-\hat{b}_4 a_{4,3} a_{3,1} b_2 c_2 - \hat{b}_4 a_{4,2} a_{2,1} b_3 c_3 - \hat{b}_2 a_{2,1} b_4 a_{4,3} c_3 - \hat{b}_3 a_{3,2} a_{2,1} b_4 c_4 + b_3 a_{3,1} \hat{b}_4 a_{4,2} c_2 - \hat{b}_3 a_{3,1} b_4 a_{4,2} c_2 - \hat{b}_4 a_{4,3} a_{3,2} a_{2,1} + b_4 a_{4,2} a_{2,1} \hat{b}_3 c_3 - \hat{b}_1 b_4 a_{4,3} a_{3,2} c_2 \\ &+ b_4 a_{4,1} \hat{b}_3 a_{3,2} c_2 - \hat{b}_4 a_{4,1} b_3 a_{3,2} c_2 + b_4 a_{4,3} a_{3,2} a_{2,1} + b_1 \hat{b}_4 a_{4,3} a_{3,2} c_2 + b_3 a_{3,2} a_{2,1} \hat{b}_4 c_4 + b_4 a_{4,3} a_{3,1} \hat{b}_2 c_2 + b_2 a_{2,1} \hat{b}_4 a_{4,3} c_3) z^8 \\ &+ (-b_4 a_{4,3} a_{3,1} - b_3 a_{3,2} a_{2,1} - b_4 a_{4,2} a_{2,1} - b_4 a_{4,3} a_{3,2} - b_1 \hat{b}_4 a_{4,2} c_2 - b_1 \hat{b}_3 a_{3,2} c_2 - b_3 \hat{b}_4 a_{4,2} c_2 + \hat{b}_2 b_4 a_{4,3} c_3 - b_2 a_{2,1} \hat{b}_3 c_3 - b_2 a_{2,1} \hat{b}_4 c_4 - b_4 a_{4,1} \hat{b}_3 c_3 \\ &- b_4 a_{4,1} \hat{b}_2 c_2 - b_4 a_{4,2} \hat{b}_3 c_3 + \hat{b}_3 a_{3,2} b_4 c_4 + \hat{b}_4 a_{4,1} b_3 c_3 + \hat{b}_4 a_{4,1} b_2 c_2 + \hat{b}_4 a_{4,2} b_3 c_3 - b_2 \hat{b}_4 a_{4,3} c_3 + \hat{b}_2 a_{2,1} b_4 c_4 + \hat{b}_3 a_{3,1} b_4 c_4 + \hat{b}_3 a_{3,1} b_2 c_2 - b_3 a_{3,1} \hat{b}_4 c_4 \\ &- b_3 a_{3,1} \hat{b}_2 c_2 - b_4 a_{4,3} \hat{b}_2 c_2 - b_3 a_{3,2} \hat{b}_4 c_4 - b_4 \hat{b}_3 a_{3,2} c_2 - b_1 \hat{b}_4 a_{4,3} c_3 + \hat{b}_4 b_3 a_{3,2} c_2 + \hat{b}_1 b_4 a_{4,3} c_3 + \hat{b}_4 a_{4,3} b_2 c_2 + \hat{b}_1 b_4 a_{4,2} c_2 + \hat{b}_1 b_3 a_{3,2} c_2 \\ &+ \hat{b}_3 b_4 a_{4,2} c_2 + \hat{b}_2 a_{2,1} b_3 c_3 + \hat{b}_3 a_{3,2} a_{2,1} + \hat{b}_4 a_{4,3} a_{3,1} + \hat{b}_4 a_{4,2} a_{2,1} + \hat{b}_4 a_{4,3} a_{3,2} - \hat{b}_4 a_{4,3} a_{3,2} c_2) z^6 \\ &+ (-\hat{b}_4 b_3 c_3 + b_4 \hat{b}_2 c_2 - \hat{b}_2 b_4 c_4 - \hat{b}_3 b_4 c_4 + b_2 \hat{b}_4 c_4 + b_3 \hat{b}_2 c_2 + b_3 \hat{b}_4 c_4 - \hat{b}_1 b_3 c_3 + b_4 \hat{b}_3 c_3 + b_1 \hat{b}_3 c_3 - \hat{b}_4 b_2 c_2 - \hat{b}_1 b_2 c_2 - \hat{b}_1 b_4 c_4 + b_1 \hat{b}_2 c_2 + b_2 \hat{b}_3 c_3 + b_1 \hat{b}_4 c_4 - \hat{b}_3 b_2 c_2 - \hat{b}_2 b_3 c_3 \\ &- \hat{b}_2 a_{2,1} - \hat{b}_3 a_{3,1} - \hat{b}_3 a_{3,2} - \hat{b}_4 a_{4,1} - \hat{b}_4 a_{4,2} - \hat{b}_4 a_{4,3} + b_2 a_{2,1} + b_4 a_{4,1} + b_4 a_{4,2} + b_3 a_{3,1} + b_4 a_{4,3} + b_3 a_{3,2} + \hat{b}_3 a_{3,2} c_2 + \hat{b}_4 a_{4,3} c_3 + \hat{b}_4 a_{4,2} c_2) z^4 \\ &+ (-b_2 - \hat{b}_4 c_4 + \hat{b}_2 - b_4 + \hat{b}_1 + \hat{b}_3 - \hat{b}_2 c_2 - b_1 - b_3 - \hat{b}_3 c_3 + \hat{b}_4) z^2 \end{aligned}$$

where $z = \nu h$

As it has already been defined, in order to have phase-lag of order infinity, the following relation must hold:

$$\Phi(z) = z - arccos\Big(\frac{R(z^2)}{2\sqrt{Q(z)^2}}\Big) = 0 \qquad (14)$$

By applying $R(z^2)$ and $Q(z^2)$ to the formula of the direct calculation of the phase lag (12) and substituting the following coefficients that have been used by Dormand et al. in [1] :

$$\begin{aligned}
\alpha_{21} &= \frac{1}{32}, \qquad \alpha_{31} = \frac{7}{1000}, \qquad \alpha_{32} = \frac{119}{500}, \qquad \alpha_{41} = \frac{1}{14}, \qquad \alpha_{42} = \frac{8}{27},\\
c_2 &= \frac{1}{4}, \qquad c_3 = \frac{7}{10}, \qquad c_4 = 1,\\
b_1 &= \frac{1}{14}, \qquad b_2 = \frac{8}{27}, \qquad b_3 = \frac{25}{189}, \qquad b_4 = 0,\\
\hat{b}_1 &= \frac{1}{14}, \qquad \hat{b}_2 = \frac{32}{81}, \qquad \hat{b}_3 = \frac{250}{567}, \qquad \hat{b}_4 = \frac{5}{54},
\end{aligned}$$

After satisfying relation (14), we have:

$$\begin{aligned}
\Phi(z) &= z - arcoss\Big(\frac{R(z^2)}{2\sqrt{Q(z)^2}}\Big) = 0 \Rightarrow\\
a_{4,3} &= -\frac{5}{5292}\frac{1}{289z^4 - 6800z^2 + 40000z^4}(54621\, z^8 - 4793320\, z^6 + 99172960\, z^4\\
&+ 5179680\, z^4 (\sin(z))^2 - 768268800\, z^2 + 4043520\, z^2 (\sin(z))^2\\
&+ 1866240000 - 559872000\, (\sin(z))^2 + 24\,(-654383577600\, z^6\\
&+ 212348252160000\, z^4 - 1366377865200\, z^8 - 1710031785\, z^{12}\\
&+ 89285428680\, z^{10} - 202307339750400\, z^4 (\sin(z))^2\\
&+ 2023399802880000\, z^2 (\sin(z))^2 - 2015539200000000\, z^2\\
&+ 581660870400\, z^6 (\sin(z))^2 + 1319799592800\, z^8 (\sin(z))^2\\
&+ 1710031785\, z^{12} (\sin(z))^2 - 89285428680\, z^{10} (\sin(z))^2\\
&+ 46578272400\, z^8 (\sin(z))^4 + 72722707200\, z^6 (\sin(z))^4\\
&- 10040912409600\, z^4 (\sin(z))^4 + 544195584000000\, (\sin(z))^4\\
&- 7860602880000\, z^2 (\sin(z))^4 + 6046617600000000\\
&- 6590813184000000\, (\sin(z))^2)^{1/2}) \qquad (15)
\end{aligned}$$

The Taylor expansion series for $a_{4,3}$, which is given from the above formula is :

$$\begin{aligned} a_{4,3} &= \frac{25}{189} - \frac{43}{2400}\,z^2 - \frac{1531}{30240000}\,z^4 - \frac{3273029}{36288000000}\,z^6 \\ &+ \frac{59772887431}{9699782400000000}\,z^8 + \cdots . \end{aligned} \tag{16}$$

## 4. Numerical examples

In this section we will apply our method to three problems. We are going to compare our results with those derived by using the high order method of embedded Runge-Kutta-Nyström 4(3)4 method of *Dormand and Prince (see [1])*.

One way to measure the efficiency of the method is to compute the accuracy in the decimal digits, that is $-log_{10}$(*maximum error through the integration intervals*)

$acc(T) = -log_{10}(max|u(t_n) - u_n|), \quad where \quad t_n = 1 + nh, \quad n = 1, 2, \ldots, \frac{T-1}{h}$ and $u(t)$ is the vector of the solution.

Table 2 shows the accuracy for the two methods. In our computations we have two step values, for Problems 1 and 2, $h = 0.025$ and $h = 0.050$, and for Problems 3 and 4, $h = 0.25$ and $h = 0.50$.

***Problem 1.*** *(Inhomogeneous equation)*

$$\frac{d^2u(t)}{dt^2} = -\nu^2 u(t) + (\nu^2 - 1)sin(t), \qquad u(0) = 1, \quad u'(0) = \nu + 1,$$

where $t \geq 0$ and $\nu = 10$.
The analytical solution is $u(t) = cos(\nu t) + sin(\nu t) + sin(t)$

***Problem 2.*** *(Two-Body problem)*

$$u'' = -\frac{u}{(u^2 + z^2)^{3/2}}, \quad z'' = -\frac{z}{(u^2 + z^2)^{3/2}}$$

where $\quad u(0) = 1, \quad u'(0) = 0, \quad z(0) = 0, \quad z'(0) = 1 \ \ and \ \ \nu = 1$

| | Our method | | | Dormand and Prince method | | |
|---|---|---|---|---|---|---|
| | T=100 | T=1000 | T=5000 | T=100 | T=1000 | T=5000 |
| *Problem 1* | | | | | | |
| h=0.025 | 4.2 | 3.2 | 2.5 | 2.3 | 1.3 | 0.6 |
| h=0.050 | 2.7 | 1.7 | 1.0 | 1.1 | 0.2 | -0.3 |
| *Problem 2* | | | | | | |
| h=0.025 | 7.3 | 5.9 | 4.6 | 6.5 | 5.1 | 3.8 |
| h=0.050 | 6.0 | 4.4 | 3.1 | 5.2 | 3.6 | 2.3 |
| *Problem 3* | | | | | | |
| h=0.25 | 5.7 | 5.4 | 5.4 | 4.2 | 4.1 | 4.1 |
| h=0.50 | 4.2 | 3.9 | 3.9 | 2.9 | 2.8 | 2.8 |
| *Problem 4* | | | | | | |
| h=0.25 | 5.2 | 4.3 | 3.4 | 3.5 | 2.5 | 1.6 |
| h=0.50 | 3.8 | 2.8 | 1.9 | 2.3 | 1.8 | 0.4 |

Table 2: Accuracy for the maximum absolute error for problems 1-4

The analytical solution is $u(t) = cos(t) \quad and \quad z(t) = sin(t)$

***Problem 3.*** *(Duffing equation)*

$$\frac{d^2u(t)}{dt^2} = -u(t) - (u(t))^3 + Bcos(\nu t)$$

where $B = 0.002$ and $\nu = 1.01$.
The analytical solution is $u(t) = A_1cos(\nu t) + A_3cos(3\nu t) + A_5cos(5\nu t) + A_7cos(7\nu t) + A_9cos(9\nu t)$
where $A_1 = 0.200179477536$, $A_3 = 0.000246946143$, $A_5 = 0.000000304014$, $A_7 = 0.000000000374$ and $A_9 = 0.000000000000$

***Problem 4.*** *(Franco and Palacios problem)*

$$\frac{d^2u(t)}{dt^2} = -u(t) + \epsilon exp(it), \qquad u(t) \in C \quad u(0) = 1, \quad u'(0) = (1 - \frac{1}{2}\epsilon)i,$$

where $\epsilon = 0.001$ and $\nu = 1$
The analytical solution is $u(t) = cos(t) + \frac{1}{2}\epsilon tsin(t) + i[sin(t) - \frac{1}{2}\epsilon tcos(t)]$

## 5. Conclusion

A new fourth order Runge-Kutta-Nyström method with phase-lag of order infinity is developed in the present paper. The new method is based on the very well known classical Dormand and Prince fourth algebraic order Runge-Kutta-Nystöm method. The numerical results show that the new method is much more efficient for integrating second-order equations with periodic oscillating behavior than the classical one.

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